GaAs-based dilute bismide semiconductor lasers: theory vs. experiment

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Abstract*—We present a theoretical analysis of the electronic and optical properties of near-infrared dilute bismide quantum well (QW) lasers grown on GaAs substrates. Our theoretical model is based upon a 12-band k·p Hamiltonian which explicitly incorporates the strong Bi-induced modifications of the band structure in pseudomorphically strained $GaBi_xAs_{1-x}$ alloys. We outline the impact of Bi on the gain characteristics of ideal $GaBi_xAs_{1-x}$/(Al)GaAs devices, compare the results of our theoretical calculations to experimental measurements of the spontaneous emission (SE) and optical gain – a first for this emerging material system – and demonstrate quantitative agreement between theory and experiment. Through our theoretical analysis we further demonstrate that this novel class of III-V semiconductor alloys has strong potential for the development of highly efficient GaAs-based semiconductor lasers which promise to deliver uncooled operation at 1.55 μm.

I. Introduction

Interest in dilute bismide alloys – in which a small fraction of the group-V atoms in a conventional III-V semiconductor are replaced by bismuth (Bi) – has been steadily increasing in recent years. The growing interest in these "highly-mismatched" materials is due to fundamental interest in the unusual properties of dilute bismide alloys, as well as their potential for specific device applications. Of particular interest is the exploitation of the effects of Bi incorporation to facilitate band structure engineering in semiconductor lasers [1]–[4].

The replacement of As by Bi to form $GaBi_xAs_{1-x}$ causes a rapid reduction of the band gap (E_g), as well as a strong increase in the spin-orbit-splitting energy (Δ_{SO}), both of which are characterised by strong, composition-dependent bowing arising from the impurity-like behaviour of substitutional Bi atoms. The incorporation of $>$ 10% Bi produces a band structure in which $\Delta_{SO} > E_g$, which offers the possibility to suppress the non-radiative (Auger) recombination and inter-valence band absorption loss mechanisms which dominate the threshold current and degrade the temperature stability of conventional InP-based QW lasers operating at telecommunication wavelengths [3].

Despite difficulties associated with the growth of Bi-containing alloys, significant progress has been made in developing dilute bismide materials and devices. Refinement of growth techniques has led to the development of electrically pumped dilute bismide QW lasers [5] which, from a theoretical perspective, has mandated the development of models of the electronic and optical properties of Bi-containing nanostructures. Here, we (i) provide an overview of the theoretical approach we have developed to study dilute bismide alloys, (ii) identify key trends relating to the impact of Bi incorporation on the properties of $GaBi_xAs_{1-x}$ QW lasers, and (iii) demonstrate how Bi incorporation can be exploited to deliver highly efficient semiconductor lasers operating at 1.55 μm.

This work was supported by the Engineering and Physical Sciences Research Council, U.K. (project nos. EP/K029665/1, EP/H005587/1 and EP/H050787/1), by the European Union (project no. FP7-257974), and by Science Foundation Ireland (project no. 10/IN.1/I2994).

II. Theoretical model

Our theoretical description of the $GaBi_xAs_{1-x}$ band structure is based upon a 12-band **k**·**p** Hamiltonian, which we have derived directly using atomistic supercell calculations [6]. This extended basis Hamiltonian directly incorporates Bi composition dependent interactions between the valence band edge states of the GaAs host matrix, and localised Bi-related impurity states. This model has been parametrised directly on the basis of ordered alloy supercell calculations [6], and we have more recently refined and constrained the Bi-related band structure parameters by comparing the band offsets and transition energies calculated using the 12-band model to the results of polarisation-resolved photovoltage measurements on a series of $GaBi_xAs_{1-x}$/(Al)GaAs QW laser structures [7].

Our calculations for QW heterostructures employ a numerically efficient plane wave approach, which provides a robust and flexible framework in which to analyse the electronic and optical properties. In our model, the material gain spectrum at fixed carrier density is computed by transforming the SE spectrum. The resulting thermodynamic consistency means that each current density (J) in experiment can be associated directly with a carrier density (n) in the theoretical calculations, thereby facilitating direct comparison between theory and experiment [8], [9]. Key to our computation of the optical spectra is the direct use of the QW eigenstates, so that the crucial effects of Bi-induced hybridisation and epitaxial strain are accounted for explicitly. (See Ref. [8] for details.)

III. Results

Firstly, we have used our theoretical model to identify and quantify trends in the gain characteristics of ideal

$GaBi_xAs_{1-x}$/(Al)GaAs QW lasers as a function of Bi composition x. Our calculations indicate that Al incorporation in the barrier layers is required for Bi compositions $< 6\%$ in order to mitigate the low $GaBi_xAs_{1-x}$/GaAs conduction band offset and bring about appreciable material gain. This leads to a trade-off between the carrier and optical confinement, which can be engineered to minimise the threshold current density [8]. As x is increased, the beneficial effects of compressive strain on the band structure dominate. We calculate that ideal $GaBi_xAs_{1-x}$ QWs designed to emit at 1.55 μm ($x \approx 13\%$) have intrinsicially superior gain characteristics than at lower x, leading to reduced threshold carrier densities and enhanced differential gain. (See Ref. [8] for details.)

Secondly, we have performed a detailed comparison between theory and experiment for $GaBi_xAs_{1-x}$/(Al)GaAs QW lasers at low x. For the experimental analysis, multi-section devices were fabricated and measurements of the SE and optical gain spectra were undertaken using the segmented contact method. By comparing the measured and calculated SE spectra, we have determined that (i) the spectral broadening is best described using a hyperbolic secant lineshape, and (ii) the large spectral linewidth, $\delta = 25$ meV, is relatively independent of temperature, indicating strong inhomogeneous broadening associated with Bi-related alloy disorder [7], [8].

Fig. 1 shows the measured (open circles) and calculated (solid lines) net modal gain spectra at several current densities for a single QW device containing 1.8% Bi, similar to that described in Ref. [5]. The theoretical gain spectra were computed as $\Gamma g - \alpha_i$ where the material gain g and optical confinement factor Γ were calculated directly for the laser structure [8], and the internal (cavity) losses $\alpha_i = 15$ cm^{-1} were extracted from optical absorption measurements [9]. In order to compare the measured and calculated spectra, analysis of the measured gain spectrum at each J was undertaken in order to extract a corresponding carrier density n to be used in the theoretical calculations [9]. We note that the calculated gain spectra are in quantitative agreement with experiment, confirming the accuracy of the theoretical model we have developed for dilute bismide semiconductor lasers. (See Ref. [9] for details.)

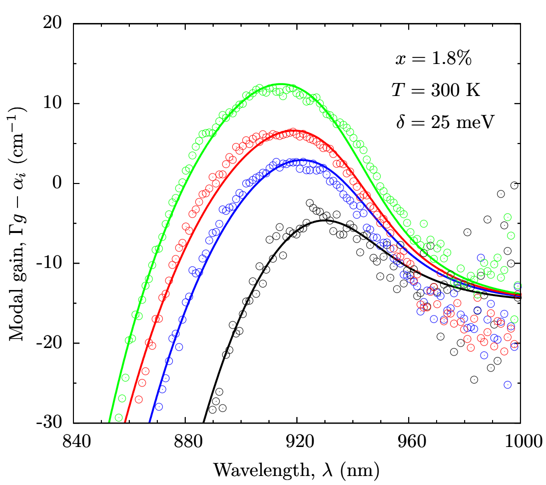

Fig. 1. Measured (open circles) and calculated (solid lines) net modal gain spectra for a $GaBi_xAs_{1-x}$/(Al)GaAs single QW diode laser with $x = 1.8\%$. The measurements were performed at current densities $J = 0.4$, 1.4, 2.0 and 2.4 kA cm^{-2}, corresponding in the theoretical calculations to carrier densities $n = 5.12$, 7.11, 8.24 and 9.38 $\times$ 10^{18} cm^{-3}. (See Ref. [9] for details.)

IV. Conclusion

Starting from a 12-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for $GaBi_xAs_{1-x}$ alloys we have developed a theoretical model of the electronic and optical properties of dilute bismide nanostructures, and have applied this model to investigate the properties and performance of GaAs-based dilute bismide QW lasers. Our analysis has (i) elucidated the impact of Bi incorporation on the electronic and optical properties, (ii) identified and quantified key trends in the performance of ideal devices as a function of Bi composition, and (iii) provided guidelines for the development of optimised devices.

We have compared the results of our calculations to experimental measurements of the SE and optical gain spectra performed on first generation $GaBi_xAs_{1-x}$ devices – the first such measurements and comparison for this emerging class of semiconductor alloys. Our calculations are in quantitative agreement with experiment, validating our theoretical model and demonstrating its promise for use in the analysis and design of photonic devices incorporating dilute bismide alloys. Overall, our analysis confirms that $GaBi_xAs_{1-x}$/GaAs QWs are a promising candidate material system for the development of highly efficient, next-generation semiconductor lasers for applications in optical communications.

Acknowledgment

The authors thank Dr. P. Ludewig and Prof. Dr. K. Volz, Philipps-Universität Marburg, Germany, for providing laser devices to facilitate the experiments, and for useful discussions.

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